

Motional effects of single trapped atomic/ionic qubit

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We investigate theoretical decoherence effects of the motional degrees of freedom of a single trapped atomic/ionic electronically coded qubit. For single bit rotations from a resonant running wave laser field excitation, we found the achievable fidelity to be determined by a single parameter characterized by the motional states. Our quantitative results provide a useful realistic view for current experimental efforts in quantum information and computing.

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Since the pioneering work by Shor [1] on efficient prime factorization with a quantum computer in 1994, we have witnessed an explosive growth of interests in quantum information and computing. Although still largely a theoretical field, solid progress in experimental efforts have been made within the last few years. Most notably, pure state based quantum gate implementation [2], demonstrations of quantum teleportation [3], and GHZ state synthesis [4] have stimulated more vigorous experimental efforts.

Two of the most interesting proposals for potentially large scale quantum computing were suggested by the same Innsbruck group, based on trapped ions [5] and cavity QED with atoms [6]. Various implementations of these ideas are actively pursued in many experiments around the world. In their original analysis as presented in [5,6], individual qubits are coded in electronic degrees states of atoms/ions, and coherent evolution of the system state requires the qubits to be in selected motional pure states. Experimentally, one needs to attain the strong binding limit [7] and cooling to the motional ground state is also required [8]. As is well known, these limits are difficult to maintain due to various decoherence processes [9] which heat up the motional degrees of freedom. Further more, maintaining motional ground state becomes problematic when strong confinement is not satisfied. Several ideas were proposed recently for computing with ‘hot’ qubits [10].

This paper attempts to provide quantitative answers to motional effects (ME) on electronically encoded quantum states [11]. It is the first step towards a thorough investigation of the ME. The paper is organized as follows. First our model is presented. We then discuss analytically the decoherence of the ME for an unknown electronic encoded qubit. Finally we present numerical results to support our understanding. In forthcoming papers, we will study the decoherence due to ME on multi-qubit entanglement creation, e.g, the effect on the conditional logic operation CNOT.

We consider a single harmonically bound two state atom described by the Hamiltonian [12–14]

$$H = \sum_{\vec{n}} \hbar (n_x \omega_x^g + n_y \omega_y^g + n_z \omega_z^g) |g, \vec{n}\rangle \langle g, \vec{n}|$$

$$\begin{aligned}
& + \sum_{\vec{m}} \hbar(\omega_{eg} + m_x\omega_x^e + m_y\omega_y^e + m_z\omega_z^e) |e, \vec{m}\rangle \langle e, \vec{m}| \\
& + \frac{1}{2} \hbar \Omega_L e^{i\omega_L t} \sum_{\vec{n}, \vec{m}} \eta_{\vec{n}\vec{m}}(\vec{k}_L) |g, \vec{n}\rangle \langle e, \vec{m}| + h.c. . \quad (1)
\end{aligned}$$

$|g, \vec{n}\rangle = |g\rangle |\vec{n}\rangle_g$ ($|e, \vec{m}\rangle = |e\rangle |\vec{m}\rangle_e$) denotes number state in the ground (excited) trap with frequencies are $\omega_{i=x,y,z}^g$ (ω_i^e). ω_{eg} is the electronic transition frequency. Ω_L is the Rabi frequency of the plane wave laser field. The motional dipole moments are the familiar Franck-Condon factor [17]

$$\eta_{\vec{n}\vec{m}}(\vec{k}_L) = \langle g, \vec{n} | e^{-i\vec{k}_L \cdot \vec{R}} | e, \vec{m} \rangle. \quad (2)$$

Radiative coupling to the vacuum reservoir of the atom will not be included here as the effect of the resulting spontaneous emission on the qubit decoherence has been studied and is well understood [5,6,10,15]. Our model can also be viewed as between two ground states in a three level Λ -type off resonant Raman system. In such a case, $\Omega_L \sim \Omega_P \Omega_S^* / \delta_L$ are the two photon effective Rabi frequency and $\vec{k}_L = \vec{k}_P - \vec{k}_S$. The indices P and S denote the dipole connected pump and stokes transitions, and δ_L is the (large) detuning from the eliminated far off-resonant excited state.

Physical models similar to Eq. (1) have been studied under different context before [5,7,13,14,16], usually, within the Lamb-Dicke limit (LDL) when ME become considerably simplified. In terms of the trap width $a_i^{g,e} = \sqrt{\hbar/2M\omega_i^{g,e}}$, the LDL corresponds to $k_L a_i^{g,e} \ll 1$. This requires the atom/ion to be confined less than the wavelength $a_i^{g,e} \ll \lambda_L$ and is equivalent to require $\hbar\omega_i^g$ to be much larger than the recoil energy $E_R = \hbar^2 k_L^2 / 2M \ll \hbar\omega_i^{e,g}$. For an effective two state system reduced from a near resonant three level Λ -type configuration, LDL is easily satisfied with co-propagating pump and Stokes fields when $\vec{k}_P \sim \vec{k}_S$.

In this study we investigate ME for general cases not in the LDL. Such studies will provide much needed theoretical clarification as trapped atoms/ions are among the “hottest” qubit candidates in many experimental efforts. We note Franck-Condon factors (2) satisfy

$$\begin{aligned}
& \sum_{\vec{n}} [\eta_{\vec{n}\vec{m}}(\vec{k}_L)]^* \eta_{\vec{n}\vec{m}'}(\vec{k}_L) = \delta_{\vec{m}\vec{m}'}, \\
& \sum_{\vec{m}} [\eta_{\vec{n}\vec{m}}(\vec{k}_L)]^* \eta_{\vec{n}'\vec{m}}(\vec{k}_L) = \delta_{\vec{n}\vec{n}'}, \quad (3)
\end{aligned}$$

which allows the introduction of a complete and orthonormal basis [17]

$$|\vec{n}\rangle_p = \sum_{\vec{n}'} \eta_{\vec{n}\vec{n}'}^*(\vec{k}_L) |\vec{n}'\rangle_g. \quad (4)$$

Physically it corresponds to the motional wave packet of a photon absorption from ground state $|\vec{n}\rangle_g$. Mathematically, it is the number coherent state basis $|\alpha, n\rangle =$

$D(\alpha)|n\rangle$, with the displacement operator $D(\alpha) = e^{\alpha b^\dagger - \alpha^* b}$. We note $R_i = a_i^g(b_i^{g+} + b_i^g)$ with b_i^g (b_i^{g+}) the annihilation (creation) operator for $|n_i\rangle_g$, therefore Eq. (4) can be rewritten as $|n_x\rangle_p = |ik_L a_x^g, n_x\rangle_g$, exactly representing wave-packets corresponding to excitation from different ground trapping states. As will become clear later, the coherent Rabi coupling between the ground and excited state manifolds can also be decomposed into paired sets $\{|g\rangle|\vec{n}\rangle_g, |e\rangle|\vec{n}\rangle_p\}$.

With the inverse relation

$$|\vec{m}\rangle_e = \sum_{\vec{n}} \eta_{\vec{n}\vec{m}}(\vec{k}_L)|\vec{n}\rangle_p, \quad (5)$$

we can transform Eq. (1) into the $|\vec{n}\rangle_p$ basis. Denote $|e_p, \vec{n}\rangle = |e\rangle|\vec{n}\rangle_p$, we obtain

$$\begin{aligned} \sum_{\vec{m}} \hbar\omega_{eg}|e, \vec{m}\rangle\langle e, \vec{m}| &= \sum_{\vec{n}} \hbar\omega_{eg}|e_p, \vec{n}\rangle\langle e_p, \vec{n}|, \\ \sum_{\vec{m}, i} m_i \hbar\omega_i^e |\vec{m}\rangle_e \langle \vec{m}| &= \sum_{\vec{n}, \vec{n}'} (E_{\vec{n}\vec{n}'}^D + E_{\vec{n}\vec{n}'}^O) |\vec{n}\rangle_p \langle \vec{n}'|. \end{aligned} \quad (6)$$

We found $E_{\vec{n}\vec{n}'}^D$ terms couple nearest neighbors, i.e. states with $n_i = n'_i \pm 1$ ($n_{j \neq i} = n'_j$), while $E_{\vec{n}\vec{n}'}^O$ terms couple states with $\vec{n} = \vec{n}'$ and $n_i = n'_i \pm 2$ ($n_{j \neq i} = n'_j$). $E_{\vec{n}\vec{n}'}^O$ terms become diagonal along i -axis whenever $\delta\omega_i^2 \neq 0$.

We will focus on the case $\omega_i^g = \omega_i^e$ ($i = x, y, z$) in the present paper. This is typical for the ion trap system and can also be arranged for optical dipole traps [18]. For the plane wave excitation along the x-axis, the ME along the y and z directions are unperturbed. Our Hamiltonian Eq. (1) can simplify to a one dimensional model

$$\begin{aligned} H &= \sum_{n_x} n_x \hbar\omega_x^g |g, n_x\rangle\langle g, n_x| \\ &+ \sum_{n_x} \hbar(n_x \omega_x^g - \Delta_L) |e_p, n_x\rangle\langle e_p, n_x| \\ &+ i(k_L a_x) \sum_{n_x} \hbar\omega_x^g \sqrt{n_x + 1} |e_p, n_x + 1\rangle\langle e_p, n_x| + h.c. \\ &+ \frac{1}{2} \hbar\Omega_L \sum_{n_x} |g, n_x\rangle\langle e_p, n_x| + h.c., \end{aligned} \quad (7)$$

where transformation to the interaction picture by

$$U(t) = \exp\left(-i\hbar\omega_L t \sum_{n_x} |e_p, n_x\rangle\langle e_p, n_x|\right) \quad (8)$$

has also been made. The detuning is $\hbar\Delta_L = \hbar\omega_L - \hbar\omega_{eg} - \frac{\hbar^2 k_L^2}{2M}$, including the recoil shift.

This Hamiltonian can be graphically illustrated as in Figure 1. The paired ladder structure resembles the familiar motional state ladders in an ion trap [7]. However, in Fig. 1, the excited states are the wave-packet basis states Eq. (4). The nearest neighbor coupling is not due to the LDL approximation. Denote $H = H_0 + H_1$ with H_1

the nearest neighbor coupling term in the excited state [the third line of Eq. (7)], H_0 becomes

$$H_0 = \hbar \begin{pmatrix} \ddots & & & & \\ & \ddots & & & \\ & & n_x \omega_x^g & \frac{\Omega_L}{2} & \\ & & \frac{\Omega_L}{2} & n_x \omega_x^g - \Delta_L & \\ & & & & \ddots \end{pmatrix}, \quad (9)$$

where each 2×2 block describes the Rabi oscillation between paired states $\{|g\rangle|n_x\rangle_g, |e\rangle|n_x\rangle_p\}$ with *exactly the same* Rabi frequency $\Omega = \sqrt{\Omega_L^2 + \Delta_L^2}$. There are no differential detunings between different pairs either. With wave function coefficients $\{C_{n_x}^g, C_{n_x}^e\}$, the 2×2 oscillation is described by

$$\begin{aligned} C_{n_x}^e(\tau) &= e^{-in_x \omega_x^g \tau} [C_{n_x}^e(0) \cos \theta - i C_{n_x}^g(0) \sin \theta], \\ C_{n_x}^g(\tau) &= e^{-in_x \omega_x^g \tau} [C_{n_x}^g(0) \cos \theta - i C_{n_x}^e(0) \sin \theta], \end{aligned} \quad (10)$$

when $\Delta_L = 0$. The pulse area is $\theta(\tau) = \frac{1}{2} \int_0^\tau \Omega(t) dt$. H_0 describes the coherent evolution between paired states with a time scale given Ω . H_1 , on the other hand couples nearest neighbors of excited motional wave pack states and can causes decoherence of an electronically coded qubit. Its time scale is determined by several factors including the trap frequency ω_x^g , Lamb Dicke parameter $k_L a_x^g$, and the highest motional state number n_x^{\max} . Assuming an electronically coded unknown qubit

$$|\psi(0)\rangle = \alpha|g\rangle + \beta|e\rangle, \quad (11)$$

(normalization $|\alpha|^2 + |\beta|^2 = 1$), an arbitrary single bit rotation is achieved through a multiplication of [19]

$$e^{i\delta} \begin{pmatrix} e^{i\gamma_1} & 0 \\ 0 & e^{-i\gamma_1} \end{pmatrix} \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} e^{i\gamma_2} & 0 \\ 0 & e^{-i\gamma_2} \end{pmatrix}.$$

δ , γ_1 , γ_2 , and ϕ are parameters. With resonant Rabi coupling, our solution Eq. (10) achieves the important θ rotation corresponds to $e^{2i\gamma_1} = -i$, and $e^{2i\gamma_2} = i$. Ideally one hopes to arrive at the target state

$$|\psi(\tau)\rangle_T = (\alpha \cos \theta - i\beta \sin \theta)|g\rangle + (\beta \cos \theta - i\alpha \sin \theta)|e\rangle,$$

with the density matrix,

$$\rho_T(\tau) = I_g^T |g\rangle\langle g| + (1 - I_g^T) |e\rangle\langle e| + (I_{ge}^T |g\rangle\langle e| + h.c.), \quad (12)$$

where

$$\begin{aligned} I_g^T &= |\alpha|^2 \cos^2 \theta + |\beta|^2 \sin^2 \theta + i(\alpha\beta^* - c.c.) \sin \theta \cos \theta, \\ I_{ge}^T &= \alpha\beta^* \cos^2 \theta + \beta\alpha^* \sin^2 \theta + i(|\alpha|^2 - |\beta|^2) \sin \theta \cos \theta. \end{aligned}$$

Due to ME the electronic qubit Eq. (11) does not remain decoupled from the motional degrees of freedom. In general, it evolves within the much larger Hilbert space containing motional states. We now study two concrete examples of decoherence assuming the initial qubit in

the enlarged Hilbert space reproduces the density matrix Eq. (12), i.e. resembles a perfect qubit to the innocent bystanders unaware of the motional degrees of freedom.

First, we consider

$$|\psi(0)\rangle_{\text{tot}} = (\alpha|g\rangle + \beta|e\rangle) \otimes |\psi(0)\rangle_{\text{cm}}, \quad (13)$$

with an initial pure motional state $|\psi(0)\rangle_{\text{cm}} = \sum_{n_x} c_{n_x} |n_x\rangle_g$ ($\sum_{n_x} |c_{n_x}|^2 = 1$). Upon tracing the motional degrees of freedom, $\rho(0) = |\psi(0)\rangle\langle\psi(0)|$ is correctly reproduced. By rewriting $|\psi(0)\rangle_{\text{tot}}$ as

$$\sum_{n_x} (c_{n_x} \alpha |g\rangle |n_x\rangle_g + \sum_{n'_x} \eta_{n_x n'_x} c_{n'_x} \beta |e\rangle |n_x\rangle_p),$$

we can analytically evolve this state with H_0 to obtain

$$\rho(\tau) = I_g |g\rangle\langle g| + (1 - I_g) |e\rangle\langle e| + (I_{ge} |g\rangle\langle e| + h.c.), \quad (14)$$

with

$$\begin{aligned} I_g &= |\alpha|^2 \cos^2 \theta + |\beta|^2 \sin^2 \theta + i(\alpha\beta^* \eta^* - c.c.) \cos \theta \sin \theta, \\ I_{ge} &= i(|\alpha|^2 - |\beta|^2) \frac{1}{2} \sin 2\theta \sum_{n_x, q_x} e^{-i(n_x - q_x) \omega_x^g \tau} c_{n_x} c_{q_x}^* \eta_{q_x n_x} \\ &\quad + \alpha\beta^* \cos^2 \theta \sum_{n_x, q_x} e^{-i(n_x - q_x) \omega_x^g \tau} c_{n_x} \sum_{q'_x} \eta_{q_x q'_x}^* c_{q'_x}^* \eta_{q_x n_x} \\ &\quad + \alpha^* \beta \sin^2 \theta \sum_{n_x, q_x} e^{-i(n_x - q_x) \omega_x^g \tau} \sum_{n'_x} \eta_{n_x n'_x} c_{n'_x} c_{q_x}^* \eta_{q_x n_x}, \end{aligned}$$

where we have defined the parameter

$$\eta(k_L) = \sum_{n_x, n'_x} c_{n_x}^* \eta_{n_x n'_x} c_{n'_x}. \quad (15)$$

We see the evolution by Eq. (10) will in general not reproduce the intended density matrix Eq. (12) because of η . H_1 term is the other reason for incomplete control although its effects (when $\Omega_L \gg \omega_x^g$) can be minimized by employing a fast pulse with $\omega_x^g \tau \ll 1$. Within such a limit, or when $\omega_x^g \tau = 2\pi$, we obtain

$$\begin{aligned} I_{ge} &= i(|\alpha|^2 - |\beta|^2) \sin \theta \cos \theta \eta(k_L) \\ &\quad + \alpha\beta^* \cos^2 \theta + \alpha^* \beta \sin^2 \theta \eta(2k_L). \end{aligned} \quad (16)$$

The necessarily condition for attending a perfect fidelity of the single bit rotation is then $\eta(k_L) \equiv 1$, which can be approximately satisfied in the LDL when $k_L a_x^g \ll 1$ or in the Λ -type Raman systems with co-propagating pump and Stokes fields. As a second example, we consider the case of a thermal motional state

$$\begin{aligned} \rho_{\text{tot}}(0) &= |\psi(0)\rangle\langle\psi(0)| \otimes \rho_{\text{cm}}(0), \\ \rho_{\text{cm}}(0) &= \sum_{n_x} \rho_{n_x}^{\text{cm}} |n_x\rangle\langle n_x|, \\ \rho_{n_x}^{\text{cm}} &= (1 - e^{-\hbar\omega_x^g/k_B T}) e^{-n_x \hbar\omega_x^g/k_B T}. \end{aligned} \quad (17)$$

This is the limiting case of an ensemble average of Eq. (13) with $c_{n_x} = \sqrt{\rho_{n_x}^{\text{cm}}} e^{-i\phi_{n_x}}$ and ϕ_{n_x} a uniform random number $\in [0, 2\pi)$. The dynamics due to H_0 can

be evolved analytically and the same density matrix Eq. (14) is obtained. After averaging over $\{\phi_n\}$, we obtain

$$\begin{aligned} \langle \eta(k_L) \rangle_{\{\phi_n\}} &= \sum_{n_x} \rho_{n_x}^{\text{cm}} \eta_{n_x n_x}(k_L) \\ &= \exp \left[-\frac{1}{2} (k_L a_x)^2 \coth \left(\frac{1}{2} \frac{\hbar \omega_x^g}{k_B T} \right) \right]. \end{aligned} \quad (18)$$

In the low temperature limit when $k_B T < \hbar \omega_x^g$, η becomes 1 as long as LDL $k_L a_x^g \ll 1$ is satisfied. At high temperatures when $k_B T \gg \hbar \omega_x^g$, $(k_L a_x^g)^2 \ll \hbar \omega_x^g / k_B T$ needs to be satisfied for η close to 1.

We now discuss the numerical solutions. Expand the total wave-function as

$$|\psi(t)\rangle_{\text{tot}} = \sum_{n_x} [c_{n_x}^g(t) |g\rangle |n_x\rangle_g + c_{n_x}^e(t) |e\rangle |n_x\rangle_p], \quad (19)$$

we have solved the Schrödinger equation including both H_0 and H_1 . The transformation Eq. (4) greatly reduces the motional Hilbert space dimension. The perceived fidelity for the electronic coded qubit Eq. (11) under transformation Eq. (12) is

$$\mathcal{F} = \text{Tr}[\rho_T(\tau) \rho(\tau)]. \quad (20)$$

We take $\alpha = \beta = 1/\sqrt{2}$ as an example to illustrate our numerical results since similar/better fidelities are obtained with other choices. In Figure 2 we compare fidelities under arbitrary $\theta(\tau)$ rotations for two different pure states. Acceptable fidelities are obtained only for $k_L a_x^g \leq 0.3$. In general larger Ω_L / ω_x^g ratios also improved fidelity although it saturates around $\Omega_L / \omega_x^g \sim 100$. Noticeable improvements are also recorded for narrower distributions in $|c_n|^2$, e.g. in Fig. 2 initial state with $c_{n_x} = \delta_{n_x,0}$ produced better fidelity. This is a direct reflection of dephasing among different motional pair states because of their different time scales from H_0 and H_1 . The oscillatory behavior is due to dephasing caused by the Rabi oscillation between motional paired states. For comparison, we note that meaningful single bit rotations need to achieve a fidelity of 1/2, the lower limit from a random (uncontrolled) sampling of final states.

Finally we compare with thermal states for several different values of $k_B T / \hbar \omega_x^g$. Surprisingly, we found the fidelity for an initial motional thermal state is always higher than its corresponding pure state. In the temperature regime considered we found acceptable results as long as LDL is maintained. In Fig. 3, we have used $k_L a_x^g = 0.1$ and $\Omega_L = 100 (\omega_x^g)$.

In conclusion, we have performed detailed theoretical studies of the decoherence of an electronically coded atom/ion qubit due to ME. By introducing a wave packet basis in the excited state, we were able to perform considerably cleaner analysis to simplify the ME. We found that a single parameter η measures the achievable fidelity of arbitrary single bit rotations. We performed numerical calculations which demonstrates our understanding and

provided quantitative limits for experiments: the LDL is always required to maintain a high fidelity for arbitrary single bit rotations. We also found that a pure motional state is not necessarily preferred although a qubit with an initial ground motional state does give rise to the highest recorded fidelity. In actual experimental implementations, a large Ω_L is also needed to assure negligible motional dephasing during τ . One can always wait for a period $2\pi/\omega_x^g$ for subsequent single bit operations since the motional wave function then always rephases to its initial state. This study will also shed light on devising schemes for overcoming ME decoherence and error corrections in trapped atomic/ionic qubits.

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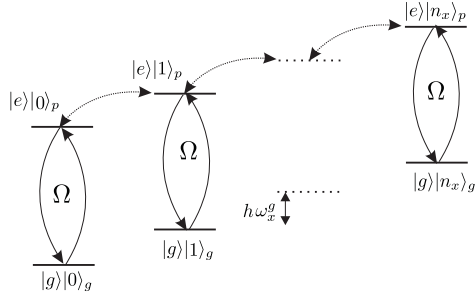


FIG. 1. The paired ladders of a trapped two state atom/ion. Solid curve arrow heads denote Rabi oscillations between paired states, while the dotted curve arrow heads denote nearest neighbor motional coupling.

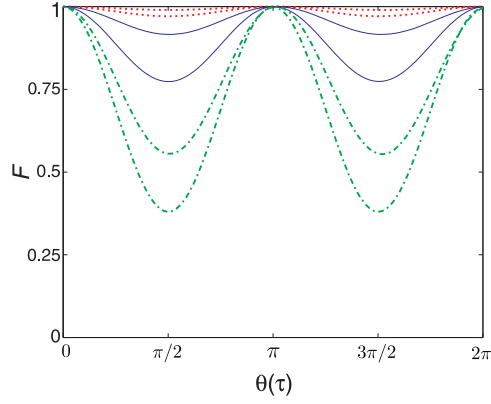


FIG. 2. The fidelity for single bit rotations with $k_L a_x^g = 0.1$ (dashed lines), 0.3 (solid lines), and 1.0 (dot dashed lines). The higher and lower fidelity sets are for initial motional state $c_{n_x} = \delta_{n_x 0}$ and $c_{n_x} = (2\delta_{n_x 0} + \sqrt{2}\delta_{n_x 1} + \delta_{n_x 2})/\sqrt{7}$ respectively. $\Omega_L = 100$ (ω_x^g).

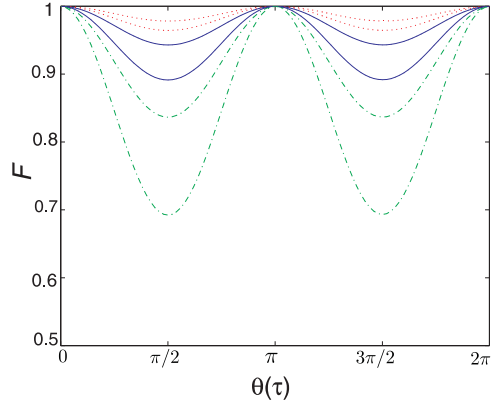


FIG. 3. The fidelity for single bit rotations with $k_B T/\hbar\omega_x^g = 1$ (dashed lines), 3 (solid lines), and 10 (dot dashed lines). The higher and lower fidelity sets are for initial motional thermal state $\rho_{n_x}^{\text{cm}}$ and pure state $c_{n_x} = \sqrt{\rho_{n_x}^{\text{cm}}}$ respectively.